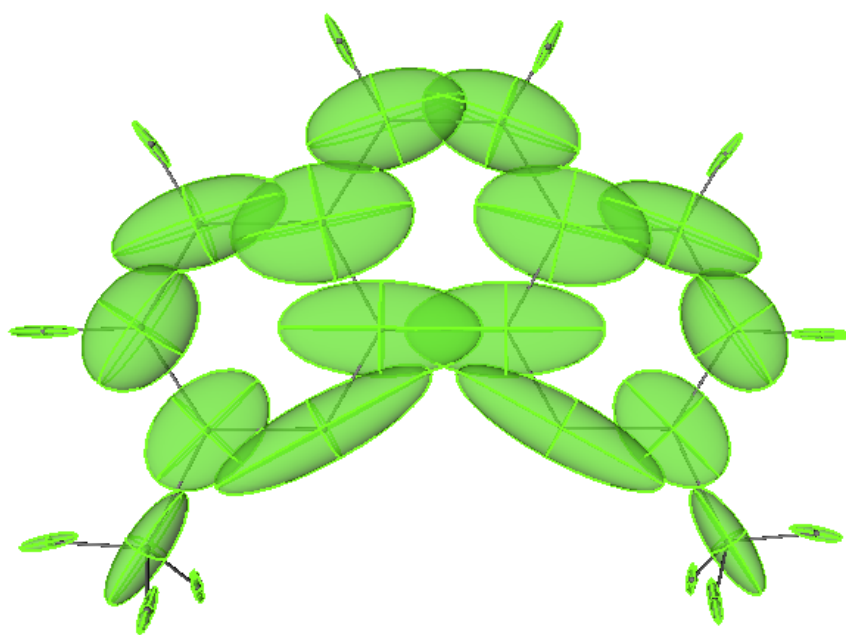


# PolaBer

Version 1.0

USER'S MANUAL

2014



## **AUTHORS:**

Anna Krawczuk  
Jagiellonian University  
krawczuk@chemia.uj.edu.pl

Piero Macchi  
University of Bern  
piero.macchi@dcb.unibe.ch

Daniel Pérez  
University of Bern

## Table of Contents

1.	INTRODUCTION .....	3
2.	LICENCE. ....	3
3.	HOW TO OBTAIN POLABER. ....	3
4.	HOW TO INSTALL POLABER. ....	3
5.	ACKNOWLEDGEMENTS.....	3
6.	INPUT CARDS .....	4
6.1	Pre-calculations .....	4
6.2	Files used and created by PolaBer .....	5
6.3	Control instructions – dipolar.inp .....	6
7.	VIEWTENSOR .....	8
7.1	Control panel / general features .....	8
7.2	Moving the molecule .....	8
7.3	Exporting files. ....	9
8.	Examples of input/output files.....	9
8.1	Control file: dipolar.inp .....	9
8.2	Format and input requests necessary for entering PolaBer (if AIMAll not used). ....	10
8.3	Output file – bond.out.....	11

## 1. INTRODUCTION

PolaBer is a program which calculates atomic polarizability tensors from electric field perturbations of a partitioned electron density distribution. Among many possible partitioning schemes PolaBer is currently interfaced with software applying quantum theory of atoms in molecules. The calculation of the atomic tensors follows the idea by Keith<sup>1</sup> that distributes over all atoms the intrinsic origin dependence of the molecular dipoles, thus increasing the possibility to export within chemical equivalent functional groups properties calculated from atomic dipoles, for example atomic polarizabilities. The software allows visualization of the tensors and calculation of straightforward optical properties of a molecule (like the molar refractive index) or a crystal (assuming the molecule in a given crystal lattice).

## 2. LICENCE.

PolaBer is a free software. You can redistribute it and/or modify it under the terms of the GNU General Public License as published by the Free Software Foundation, either version 3 of the License, or (at your option) any later version.

The software is distributed in the hope that it will be useful, but without any warranty; without even the implied warranty of merchantability or fitness for a particular purpose. See the Free Software Foundation, either version 3 of the License, or GNU General Public License for more details (<http://www.gnu.org/licenses/>).

## 3. HOW TO OBTAIN POLABER.

The program is available on request from the authors in the form of a source code or can be downloaded directly from the web site <http://www.macchi.dcb.unibe.ch>

Please do not use any output from the program without citation of the authors:

Krawczuk, A.; Perez, D.; Macchi P. (2014) *submitted*  
please check in the future on [www.macchi.dcb.unibe.ch/PolaBer.html](http://www.macchi.dcb.unibe.ch/PolaBer.html) for final publication details

Please report any bugs by e-mail to: [krawczuk@chemia.uj.edu.pl](mailto:krawczuk@chemia.uj.edu.pl) or [piero.macchi@dcb.unibe.ch](mailto:piero.macchi@dcb.unibe.ch)

## 4. HOW TO INSTALL POLABER.

On Windows XP/Vista/7/8 simply copy the folder contained in the compressed file on the PC and run viewtensor.exe (that could be linked to an icon on the desktop).

For Linux platform, sources of the code are provided (only on request) and can be compiled using the makefile available (or modifying it according to the compiler available). PolaBer is written in Fortran90 and it requires an adequate compiler (for example gfortran).

Lapack libraries must be installed as well. Static precompiled binaries are also available.

## 5. ACKNOWLEDGEMENTS.

This work was done thanks to financial support from the Swiss Conference of Rectors (CRUS) and Swiss National Science Foundation (project Nr. 141271).

---

<sup>1</sup> Keith, T.A. (2007) *Atomic Response Properties in The Quantum Theory of Atoms in Molecules: From Solid State to DNA and Drug Design*, Eds. Matta, C.F. & Boyd, R.J., Wiley-VCH, Weinheim.

## 6. INPUT CARDS

### 6.1 Pre-calculations

Since polarizabilities obtained with PolaBer are numerical derivatives of the corresponding atomic dipoles with respect to applied electric field EF, following calculations have to be carried out before entering PolaBer:

- *calculations of wave functions at zero electric field and small electric field, e.g. 0.005 a.u., directed towards  $\pm X$ ,  $\pm Y$   $\pm Z$ , respectively.*

Example of a Gaussian input file:

```
%chk=polar.chk
%Nproc=12
#b3lyp/6-311++g(2d,2p) opt out=wfn

B3LYP 6-31++G(2d,2p) H2O

0 1
O      0.000000    0.000000    0.200000
H      0.000000   -0.500000   -0.700000
H      0.000000    0.500000   -0.700000

zero.wfn
--link1--
%chk=polar.chk
%Nproc=12
#b3lyp chkbasis nosymm scf=tight geom=checkpoint out=wfn field=x+50

x=50

0 1

xp.wfn
--link1--
....
--link1--
%chk=polar.chk
%Nproc=12
#b3lyp chkbasis nosymm scf=tight geom=checkpoint out=wfn field=z-50

z=-50

0 1

zm.wfn
,
```

**Note:** If you want to calculate crystal properties (*i.e.* refractive indices or rotatory power) following steps have to be applied:

1. Export experimental fractional coordinates from a cif file to Cartesian
2. Keep *nosymm* command (when running Gaussian calculations) which will ensure no change in the definition of the coordinate system.
3. Input in PolaBer the unit cell (consistent with the coordinate setting) in order to compute crystal properties in correct form.

PolaBer gives values of atomic polarizabilities in both fractional and Cartesian coordinate systems.

- integration of electron density after expanding the molecular density in terms of multipoles.

At the moment PolaBer is compatible with AIMAll (Keith, 2013) and XD2006 (Volkov *et al.*, 2006) software.

In case of XD2006 the format of xd\_pro.out file is not recognized by PolaBer, therefore additional external routine is used to extract necessary data. The routine *xdread.exe* is available with the main code and produces new output file readable by PolaBer.

#### **xdread.exe:**

input file:      xd\_pro.out (obtained for every wave function)  
output file:      polaber.out

Other software could be used, but a generalized input files has to be created by external software. The structure and contents of input file are given in Table 6.1.

**Table 6.1** Format and input requests necessary for entering PolaBer.

Number of atoms: natoms	
At1	Atom label
xyz	Coordinates of At1 given in Å in Cartesian system
Vol	Atomic volume (calculated at $\rho = 0.001$ au) given in Å <sup>3</sup>
Q(A)	Atomic charge
Dipole	Cartesian atomic unabridged moments given in Debye/Å <sup>(l-1)</sup>
Quadrupole	
Octupole	
Hexadecapole	
Number of bonds: nbond	
At1 At2 xyz rho delrho ellips d1 d2	xyz: coordinates of BCP in Å in Cartesian system rho: electron density on BCP delrho: Laplacian of electron density on BCP Ellips: bond ellipticity d1, d2: Distances between At1 and BCP and BCP and At2 given in Å in Cartesian system

## **6.2 Files used and created by PolaBer**

Input:

*dipolar.inp* – control file

\*.sum – output files after integration of electron density when AIMAll software is used

\*.out – output files after integration of electron density when XD2006 package is used

**Note:** Keep the format of input files as recommended.

Output:

*bond.out* – summary of calculations of atomic/bond polarizability

*bond.res* – a crystallographic format, format the same as the one produced by SHELX program (Sheldrick, 2008). Instead of ADP's, components of atomic polarizability tensors are given, scaled by the factor of 0.1  
*bond.x3d* – file for visualization in a 3D scene with ViewTensor  
*bond.x3draw* – supporting file for visualization purpose

### 6.3 Control instructions – dipolar.inp

**INTEG WEIGHT VERBOSE n**

**INTEG** specifies which program was used for integration of electron density. Currently available AIMALL/XD

**WEIGHT** if this keyword is present, weighting scheme will be used.

Weighting scheme is used to avoid drastic changes of the shape and values of atomic polarizabilities caused by a presence of weak intra- and intermolecular interactions. PolaBer uses a weighting scheme which is inversely proportional to the bond strength measured by electron density at BCP:

$$\lambda(\Omega|\Omega + 1) = \frac{1}{\rho(\Omega|\Omega + 1)}$$

**VERBOSE n** (n=0,1,2) setting n greater than 0 switches on extra printout to the output file (bond.out). By default n is set to 0.

**Nfiles**

Number of files to be read into PolaBer from AIMALL or XD software.

nfiles= 4 if calculations were done for EFIELD=0, X, Y, Z

nfiles= 7 if calculations were done for EFIELD=0, +/-X,+/-Y,+/-Z (highly recommended)

**fname1 EFIELD EFX EFY EFZ**

...

**fname EFIELD EFX EFY EFZ**

**fname** defines AIMAll (\*.sum) or XD (\*.out) filename with specification of applied electric field **EFIELD**.

Example:

If electric field is applied in X direction with the value of 0.005 au and integration of electron density was done with AIMAll software then:

xp.sum EFIELD 0.005 0. 0.

**Note:** Number of fname lines should be equal to nfiles.

**cell parameters**

<b>a</b>	<b>b</b>	<b>c</b>	<b>alpha</b>	<b>beta</b>	<b>gamma</b>
<b>esda</b>	<b>esdb</b>	<b>esdc</b>	<b>esdalpha</b>	<b>esdbeta</b>	<b>esdgamma</b>

Cell parameters given in Å and deg in fractional coordinates with their esds.

**LATT N**

**LATT** defines lattice type following SHELX convention:

$N=1-7$

1=P, 2=I, 3=R<sub>0bv</sub> on hexagonal axes, 4=F, 5=A, 6=B, 7=C negative sign indicates non-centrosymmetric structure.

**SYMM** **x1 y1 z1 x2 y2 z2 x3 y3 z3, txt y tz**

**SYMM** specifies symmetry operations given by space group

**x1 y1 z1** - 1st row of rotation matrix

**x2 y2 z2** - 2nd row of rotation matrix

**x3 y3 z3** - 3rd row of rotation matrix

**tx,ty,tz** -translational components in decimal notation +/- 0.25, 0.33, 0.5, 0.67, 0.75

Example: For space group P2<sub>1</sub>/c

```
SYMM 1 0 0 0 1 0 0 0 1, 0 0 0
SYMM -1 0 0 0 1 0 0 0 -1, 0 0.5 0.5
```

**TYPE** **n<sub>type</sub>**

**SFAC** **C H O**

**UNIT** **10 10 10**

**N<sub>type</sub>** defines number of atom types

**SFAC** responds to scattering factors for each type of atom

**UNIT** number of atoms of each type in a studied system, in SFAC order

**LAMBDA**

Gives a wavelength in Å

**ATOMLIST**

**Nlist**

**at1 at2 ...**

If a keyword **ATOMLIST** is present, additional summary table for a chosen fragment will be created in bond.out.

**nlist** gives a number of atoms to be included in a ATOMLIST table

**at1, at2** specifies atoms building chosen fragment which will be included in ATOMLIST table

<b>Note:</b> controlling file dipolar.inp is case sensitive.
--

## 6.4 Running PolaBer

To run a calculation with PolaBer open **ViewTensor**. Click on **File** and select **Run PolaBer**. After choosing a directory where all input files are present (\*.sum/\*.out and dipolar.inp), PolaBer will start the calculation of polarizabilities. When the calculation is finished, click on the button **Done**

## 6.5 Creating files for visualization

To create a file for visualization purposes, click on **File** and select **Convert Raw File**. Program will ask you for opening **X3draw** file which is present in the directory where PolaBer calculations were done. After choosing the right file program will ask you to save new x3d file in a chosen destination folder. When clicking save ViewTensor will inform you that the file was converted and by clicking **OK** the program will open the x3d file. ViewTensor uses a default view where Z axis (Cartesian system) is directed towards the viewer.

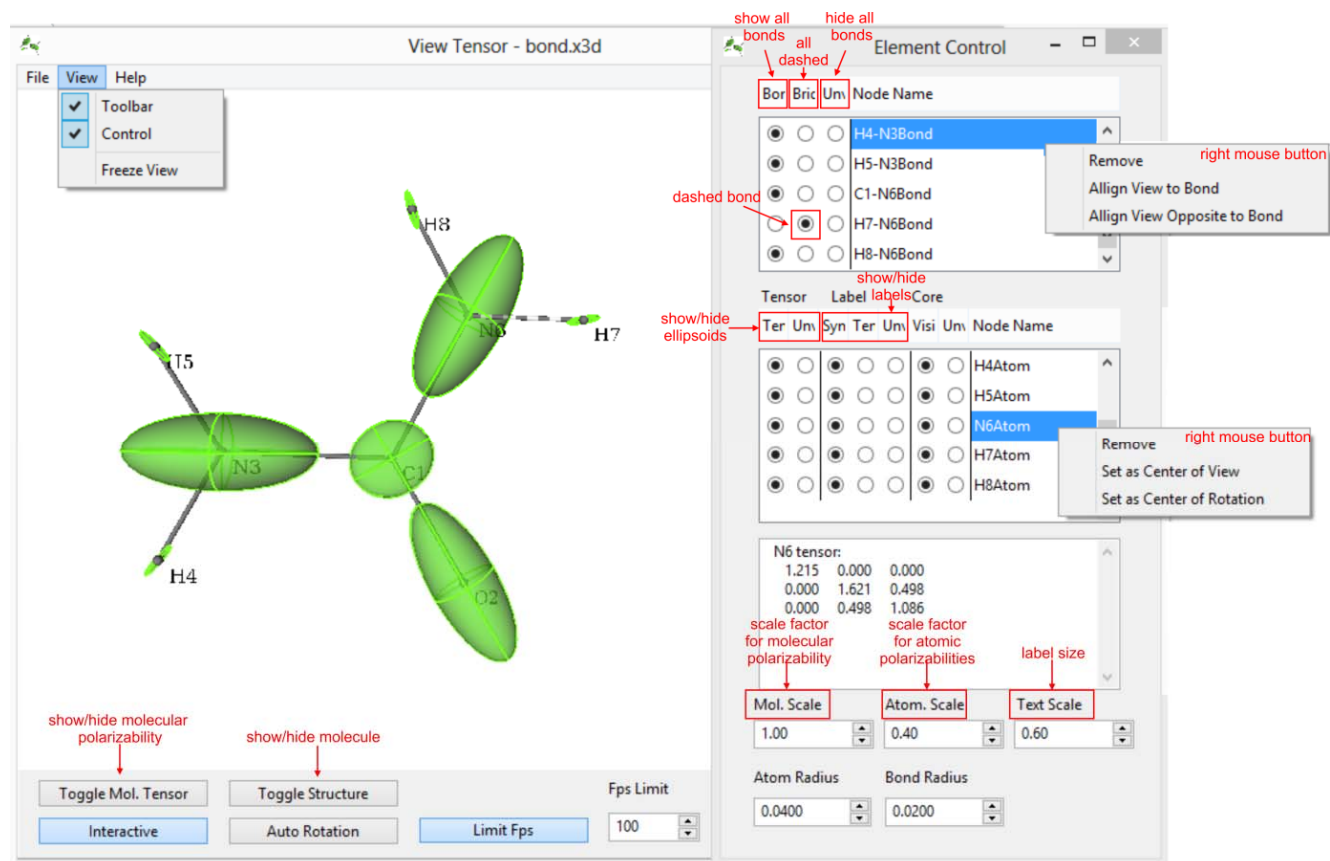
## 7. VIEWTENSOR

ViewTensor works on Windows platform and it is based on view3dscene by Kamburelis<sup>2</sup>. It generates x3d file representing data in a 3D scene. Polarizability ellipsoids are represented in the same space as the molecule, assuming that  $1\text{\AA}^3 \equiv 1\text{\AA}$ .

To open x3d file choose **File**, select **Open** and then choose the directory you were working with. After opening the x3d file a graphical representation of atomic polarizabilities in a chosen system will appear.

### 7.1 Control panel / general features

To open control panel choose **View** and select **Control**. This panel allows to configure bonds and polarizability ellipsoids in terms of style, thickness, radius and appearance. Available options on a control panel are explained in Figure 7.1. Most of the menu items intuition, but feel free to play around to find out more options.



**Figure 7.1** Screenshot of ViewTensor window. Some of the features are marked and explained in red.

### 7.2 Moving the molecule

<sup>2</sup> Kamburelis, M. (2011) view3dscene(version 3.10.1), <http://castle-engine.sourceforge.net>



To rotate a molecule keep the left mouse button pressed and move it, the molecule will rotate about the X and Y axes. To rotate molecule around Z axis use the PAGE-UP / PAGE-DOWN button. To move molecule around press and hold the middle mouse button. By pressing and holding right mouse button zoom in and zoom out the molecule.

Instead of using mouse buttons you can also use keyboard shortcuts. The list of available options is given in Table 7.2.1. To increase the speed of rotation of the molecule just hold longer control buttons. It is also possible to turn on/off the constant rotation about chosen axis. To turn on/off the constant rotation, press the Auto Rotation button on the Toolbar at the bottom of the ViewTensor window. By default Auto rotation is on.

**Table 7.2.1** Keyboard shortcuts used in ViewTensor.

Key	Function
PAGE-UP / PAGE-DOWN	rotate along Z axis
Right/left arrow	rotate along X axis
Up/down arrow	rotate along Y axis
Space bar	stop rotation
HOME	bring to default view
+/-	zoom in / zoom out;
SHIFT + left mouse button	move molecule around

### 7.3 Exporting files.

To save image choose **File -> Save Screenshot**. Save dialog appears where you can choose the name of the file and directory where the image will be saved. Two types of file format are available: .bmp and .png.

## 8. Examples of input/output files

### 8.1 Control file: dipolar.inp

---

```

AIMALL WEIGHT VERBOSE 0
7
zero.sum  EFIELD  0.      0.      0.
xp.sum     EFIELD  0.005  0.      0.
xm.sum     EFIELD  -0.005  0.      0.
yp.sum     EFIELD  0.      0.005  0.
ym.sum     EFIELD  0.      -0.005  0.
zp.sum     EFIELD  0.      0.      0.005
zm.sum     EFIELD  0.      0.      -0.005

cell parameters
10.0000 10.0000 10.0000 90.000 90.000 90.000
 0.0000 0.0000 0.0000 0.000 0.000 0.000

SYMM  1 0 0 0 1 0 0 0 1, 0.0 0.0 0.0

LATT  -1
TYPE  4
SFAC  C  H  O  N
UNIT  7  28 7  14

```

---

```

ATOMLIST
8
C1 O2 N3 H4 H5 N6 H7 H8

```

For clarity only a part of input file is showed.

ATOMIC COORDINATES GIVEN IN ANGSTROMS (ORTHOGONAL SYSTEM)  
 ATOMIC VOLUME (V001) GIVEN IN ANGSTROM^3  
 CARTESIAN ATOMIC UNABRIDGED MOMENTS GIVEN IN DEBYE-ANGSTROM^(1-1)

ATOM:	N(3)					
xyz:	0.00000000	1.16034000	-0.59564000			
VOL:	17.82578394					
Q(A):	-1.01695782					
DIPOLE:	0.00972130	-0.15982950	0.08070210			
QUADRUPOLE:	-7.78033540	0.00065970	-0.00196960	-5.77582780	0.10526430	-5.49237610
OCTUPOLE:	0.00368600	-0.34784480	0.18410040	0.00240460	0.00040740	0.00378830
	-0.85917130	0.78791460	-0.27192870	-0.19784210		
HEXADECAPOLE:	-9.37016360	-0.00006320	-0.00300160	-2.18262190	-0.04014280	-2.18257530
	0.00082670	-0.00036700	0.00024040	-0.00389300	-3.94655010	0.49898530
	-1.31687130	-0.04739350	-3.11084100			

ATOM:	H(4)					
xyz:	0.00000000	2.02238000	-0.08434000			
VOL:	4.87352353					
Q(A):	0.37531402					
DIPOLE:	-0.00364160	-0.36223760	-0.19620990			
QUADRUPOLE:	-0.45966470	-0.00069070	-0.00034190	-0.39501700	0.04358430	-0.41820410
OCTUPOLE:	-0.00246620	-0.16538950	-0.09271780	-0.00064220	0.00010910	-0.00071310
	-0.34212350	-0.00657050	-0.11580570	-0.20846130		
HEXADECAPOLE:	-0.35163640	-0.00100170	-0.00052070	-0.16287390	-0.02604890	-0.12488950
	-0.00055150	0.00007560	-0.00020020	-0.00037350	-0.47754710	0.00431420
	-0.13179050	-0.05053170	-0.32181300			

ATOM:	H(5)					
xyz:	0.00000000	1.18607000	-1.59730000			
VOL:	5.47667135					
Q(A):	0.30743514					
DIPOLE:	-0.00428030	0.00641510	0.47913380			
QUADRUPOLE:	-0.53255160	-0.00010950	0.00079940	-0.51349880	0.00445130	-0.41887560
OCTUPOLE:	-0.00290780	-0.00497510	0.21612140	-0.00090850	0.00003160	-0.00056480
	-0.04848880	0.18702320	-0.01012420	0.37460970		
HEXADECAPOLE:	-0.42270140	-0.00011150	0.00110460	-0.12941190	0.00674700	-0.19657160
	-0.00016580	0.00030770	-0.00002530	0.00040930	-0.33535720	0.04931750
	-0.16129540	0.01719780	-0.49905210			

```
xyz, d1, d2 GIVEN IN ANGSTROMS (CARTESIAN SYSTEM)
rho, delrho GIVEN IN e-/ANG^x
NUMBER OF BONDS: 7
```

[illegible]

## 8.2 Output file – bond.out

For sake of clarity only a part of the output file is listed.

-----  
POLABER - A PROGRAM FOR ATOMIC POLARIZABILITY CALCULATIONS

Anna Krawczuk; Daniel Perez; Piero Macchi (C)  
University of Bern  
Version 1.0 January 2014

-----  
ATOMIC UNITS (A.U.) USED, EXCEPT WHERE STATED OTHERWISE

UNIT CELL PARAMETERS (and e.s.d)

-----  
a,b,c given in Angstroms

-----  
          a          b          c      alpha      beta      gamma  
10.0000  10.0000  10.0000  90.0000  90.0000  90.0000  
0.0000   0.0000   0.0000   0.0000   0.0000   0.0000  
-----

SYMMETRY OPERATION

1      0      0      0.00  
0      1      0      0.00  
0      0      1      0.00

...

SYMMETRY OPERATION

0      1      0      0.00  
-1     0      0      0.00  
0      0     -1      0.00

-----  
WORKING ON: zero.sum

NUMBER OF ATOMS:                  56

-----  
NUMBER OF RINGS =                  2

TOTAL ATOMIC DIPOLE MOMENTS

-----  
symbol          x          y          z  
-----  
C1         -0.00000641     0.00029283     -0.70279781  
O2         -0.00062234     -0.00000027     -1.95720527  
N3          0.00002975      0.29284280     -0.16332389  
...  
N54         -0.24388002     -0.00006970     -0.03027765  
H55         -0.11705132      0.00004427     -0.05954688  
H56         -0.00373060      0.00000049      0.00645011  
-----

TOTAL MOLECULAR DIPOLE MOMENT

-----  
          x          y          z  
-0.00175771  0.00125971  -0.00964547  
-----

...

-----  
WORKING ON: zm.sum

NUMBER OF ATOMS:                  56

-----  
NUMBER OF RINGS =                  2

## TOTAL ATOMIC DIPOLE MOMENTS

symbol	x	y	z
C1	0.00005776	0.00011104	-0.67442148
O2	-0.00032053	0.00001327	-1.87197655
N3	0.00003513	0.27915152	-0.11798253
...			
N54	-0.25511695	-0.00009536	0.00152691
H55	-0.11551872	0.00004165	-0.05721693
H56	-0.00365758	0.00000278	0.01721425

## TOTAL MOLECULAR DIPOLE MOMENT

x	y	z
-0.00139372	0.00099155	1.41178403

## DIAGONALIZED ATOMIC POLARIZABILITY TENSORS IN CARTESIAN SYSTEM

alpha11, alpha22, alpha33 - Diagonal components of diagonalized atomic polarizability tensor  
alphaiso - Isotropic value of atomic polarizability

ATOM	alpha11	alpha22	alpha33	alphaiso
C1	2.055	5.628	7.344	5.009
O2	5.137	11.425	16.960	11.174
N3	6.244	7.925	14.015	9.395
...				
N54	5.573	6.383	14.374	8.777
H55	0.260	0.277	3.439	1.325
H56	0.442	0.588	2.244	1.091

## ATOMIC PROPERTIES

q(A) - Atom charge (EF=0)

alpha11, alpha22, alpha33, alpha12, alpha13, alpha23 - Tensor components of atomic polarizability  
alphaiso - Isotropic value of atomic polarizability

Vol - Atomic volume bounded by an isosurface of the electron density distribution (0.001 a.u. Isodensity Envelope, EF=0)

Atom	q(A)	alpha11	alpha22	alpha33	alpha12	alpha13	alpha23	alphaiso	V
C1	1.695	2.055	7.344	5.628	0.003	-0.004	-0.002	5.009	33.611
O2	-1.259	11.425	5.138	16.960	0.012	0.005	0.001	11.174	118.607
N3	-1.081	6.244	12.856	9.085	0.001	-0.006	-2.391	9.395	116.292
...									
N54	-1.099	13.532	6.383	6.415	0.010	-2.589	-0.002	8.777	118.174
H55	0.458	3.258	0.260	0.459	0.003	0.735	0.002	1.325	20.917
H56	0.359	0.615	0.442	2.217	0.000	-0.211	0.000	1.091	32.540

## MOLECULAR POLARIZABILITY TENSOR, AU^3 CARTESIAN SYSTEM

XX	YY	ZZ	XY	XZ	YZ
236.850	224.479	285.006	0.054	-0.065	0.005

## DIAGONALIZED MOLECULAR POLARIZABILITY TENSOR IN CARTESIAN SYSTEM

alpha11	alpha22	alpha33	alphaiso
140.026	203.713	402.596	248.778

MOLAR VOLUME 3597.5104

## MOLECULAR REFRACTIVE INDEX

1.3347 1.3512 1.4145

MOLECULAR RELATIVE PERMITTIVITY (dimensionless)  
71.2907

For a calculation with polarizable continuum medium in G09 use the following instructions  
SCFR=(dipole,dielectric= 71.291,a0= 5.030)

#### BOND PROPERTIES

-----  
D(A-B) - Bond lenght of A-B in au  
d1 - Distance between atom A and BCP (EF=0)  
d2 - Distance between BCP and atom B (EF=0)  
d1 + d2 = Bond path (BP)  
rho - Electron density (EF=0)  
delrho - Laplacian of electron density (EF=0)  
elips - Bond ellipticity (EF=0)  
bcharge - Bond charge (EF=0)  
polA - Projection of polarizability of atom A on A-B bond  
polB - Projection of polarizability of atom B on A-B bond  
bondpol = polA + polB  
dipA - Projection of total dipole moment of atom A on A-B bond  
dipB - Projection of total dipole moment of atom B on A-B bond  
bonddip = dipA + dipB

A-B	D(A-B)	d1	d2	rho	delrho	elips	bcharge	polA	polB	bondpol	dipA	dipB	bonddip
O2 C1	2.378	1.541	0.836	0.384	-0.910	0.076	-1.342	16.960	5.628	22.588	-1.957	-0.703	-2.660
N3 C1	2.538	1.511	1.027	0.344	-1.158	0.214	-0.176	13.955	6.875	20.829	0.335	0.369	0.704
N3 H5	1.884	1.402	0.438	0.356	-1.993	0.043	-0.446	9.014	2.591	11.605	-0.159	-0.091	-0.250
...													
H53N51	1.884	0.469	1.374	0.356	-1.804	0.056	0.361	2.512	6.728	9.240	0.005	-0.039	-0.034
N54H55	1.900	1.424	0.432	0.347	-1.971	0.046	-0.481	9.557	3.203	12.760	-0.227	-0.131	-0.358
H56N54	1.884	0.469	1.373	0.356	-1.802	0.053	0.359	2.210	6.339	8.549	0.006	-0.034	-0.028

#### ATOMIC POLARIZABILITIES FOR CHOSEN FRAGMENT

Atom	alpha11	alpha22	alpha33	alpha12	alpha13	alpha23	alpha1so
C1	2.055	7.344	5.628	0.003	-0.004	-0.002	5.009
O2	11.425	5.138	16.960	0.012	0.005	0.001	11.174
N3	6.244	12.856	9.085	0.001	-0.006	-2.391	9.395
H4	0.293	3.507	0.673	0.007	-0.006	0.980	1.491
H5	0.300	0.725	2.586	-0.004	-0.006	0.180	1.203
N6	6.243	12.852	9.073	-0.004	0.001	2.406	9.389
H7	0.301	3.512	0.678	0.007	0.003	-0.971	1.497
H8	0.303	0.730	2.584	-0.002	-0.002	-0.179	1.205

#### TOTAL POLARIZABILITY TENSOR OF A CHOSEN FRAGMENT, CARTESIAN SYSTEM, AU^3

XX	YY	ZZ	XY	XZ	YZ
27.162	46.662	47.267	0.021	-0.015	0.024

#### CRYSTAL PROPERTIES

NUMBER OF ATOMS IN THE UNIT CELL 16

#### FRACTIONAL COORDINATES OF ATOMS IN THE UNIT CELL

symbol	x	y	z
C1_1	0.0000	0.5019	0.3291
O2_1	0.0000	0.5019	0.5978
N3_1	0.1452	0.6471	0.1788
H4_1	0.2562	0.7580	0.2852
...			
H5_3	0.6452	-0.1433	0.0340
N6_3	0.3566	0.1452	-0.1788
H7_3	0.2457	0.2562	-0.2852
H8_3	0.3585	0.1433	0.0340

## NOTE:

Atoms are kept in order to form regular molecules  
and they do not necessarily lie in the unit cell  
 $0 < x < 1$ ;  $0 < y < 1$ ;  $0 < z < 1$

ATOMIC POLARIZABILITIES IN THE UNIT CELL, FRACTIONAL SYSTEM,  $\text{\AA}^3$ 

Atom	alpha11	alpha22	alpha33	alpha12	alpha13	alpha23
C1_1	0.685	0.703	0.886	0.385	0.006	0.005
O2_1	1.220	1.226	2.588	-0.463	0.011	0.010
N3_1	1.403	1.416	1.362	0.484	-0.258	-0.261
H4_1	0.278	0.285	0.099	0.235	0.097	0.099
...						
H5_3	0.078	0.079	0.394	-0.031	-0.022	0.024
N6_3	1.429	1.401	1.359	-0.489	-0.270	0.274
H7_3	0.293	0.273	0.092	-0.237	0.094	-0.088
H8_3	0.078	0.077	0.394	-0.030	0.022	-0.019

## CRYSTAL SUSCEPTIBILITY CHI

0.9453	0.0000	0.0015
0.0000	0.9453	0.0064
0.0015	0.0064	1.2416

## CRYSTAL DIELECTRIC CONSTANT EPSILON

1.9453	0.0000	0.0015
0.0000	1.9453	0.0064
0.0015	0.0064	2.2416

## REFRACTIVE INDICES

n1 &lt; n2 &lt; n3

n1	n2	n3
1.3947	1.3947	1.4972

## positive UNIAXIAL OPTICAL INDICATRIX

## BARICENTER OF MOLECULES IN UNIT CELL (FRACTIONAL COORDINATES)

Symm. Nr.	X	Y	Z
_1	0.5000	0.0000	0.2736
_3	0.0000	-0.5000	-0.2736

Please note that the selected molecules may not be within  $0 < x < 1$ ;  $0 < y < 1$ ;  
 $0 < z < 1$

## LORENTZ CORRECTION: ALFFA TYPE

## CRYSTAL SUSCEPTIBILITY CHI

1.1315	0.0000	0.0012
0.0000	1.1315	-0.0003
0.0012	-0.0003	1.5264

## CRYSTAL DIELECTRIC CONSTANT EPSILON

2.1315	0.0000	0.0012
0.0000	2.1315	0.0000
0.0012	0.0000	2.5264

## REFRACTIVE INDICES

n1 &lt; n2 &lt; n3

n1	n2	n3
1.4600	1.4600	1.5895

## positive UNIAXIAL OPTICAL INDICATRIX

-----  
RIGOROUS LOCAL FIELD THEORY

Lorentz Tensor Total  
0.3239 0.0000 0.0000  
0.0000 0.3239 0.0000  
0.0000 0.0000 0.3521  
  
Lij Trace = 1.0000

-----  
CALCULATION USING MOLECULAR POLARIZABILITIES

CRYSTAL SUSCEPTIBILITY CHI  
1.1196 0.0000 0.0012  
0.0000 1.1196 -0.0003  
0.0012 -0.0003 1.5715

CRYSTAL DIELECTRIC CONSTANT EPSILON  
2.1196 0.0000 0.0012  
0.0000 2.1196 0.0000  
0.0012 0.0000 2.5715

REFRACTIVE INDICES  
n1 < n2 < n3  
n1 n2 n3  
1.4559 1.4559 1.6036

positive UNIAXIAL OPTICAL INDICATRIX